Linear programming

Optimization Problems

- *General optimization* problem

$$\max\{z(x) \mid f_j(x) \leq 0, x \in D\} \text{ or } \min\{z(x) \mid f_j(x) \leq 0, x \in D\}$$

  where $D \subseteq \mathbb{R}^n$, $f_j : D \to \mathbb{R}$, for $j = 1, \dots, m$, $z : D \to \mathbb{R}$.

- *Linear optimization* problem

$$\max\{c^T x \mid Ax \begin{smallmatrix}\leq\\=\\\geq\end{smallmatrix} b, x \in \mathbb{R}^n\}, \text{ with } c \in \mathbb{R}^n, A \in \mathbb{R}^{m \times n}, b \in \mathbb{R}^m$$

- *Integer* optimization problem: $x \in \mathbb{Z}^n$
- *0-1* optimization problem: $x \in \{0,1\}^n$

Feasible and optimal solutions

- Consider the optimization problem

$$\max\{z(x) \mid f_j(x) \leq 0, x \in D, j = 1, \dots, m\}$$

- A *feasible solution* is a vector $x^* \in D \subseteq \mathbb{R}^n$ such that $f_j(x^*) \leq 0$, for all $j = 1, \dots, m$.
- The set of all feasible solutions is called the *feasible region*.
- An *optimal solution* is a feasible solution such that

$$z(x^*) = \max\{z(x) \mid f_j(x) \leq 0, x \in D, j = 1, \dots, m\}.$$

- Feasible or optimal solutions
  - need not exist,
  - need not be unique.

Transformations

- $\min\{z(x) \mid x \in S\} = \max\{-z(x) \mid x \in S\}$.
- $f(x) \geq a$ if and only if $-f(x) \leq -a$.
- $f(x) = a$ if and only if $f(x) \leq a \wedge -f(x) \leq -a$.

Lemma

Any linear programming problem can be brought to the form

$$\max\{c^T x \mid Ax \leq b\} \text{ or } \max\{c^T x \mid Ax = b, x \geq 0\}.$$

Proof: a) $a^T x \leq \beta \rightsquigarrow a^T x + x' = \beta, x' \geq 0$ *(slack variable)*
b) x free $\rightsquigarrow x = x^+ - x^-$, $x^+, x^- \geq 0$.

Practical problem solving

1. Model building
2. Model solving
3. Model analysis

Example: Production problem

A firm produces n different goods using m different raw materials.

- b_i: available amount of the i-th raw material
- a_{ij}: number of units of the i-th material needed to produce one unit of the j-th good
- c_j: revenue for one unit of the j-th good.

Decide how much of each good to produce in order to maximize the total revenue $\rightsquigarrow$ *decision variables x_j.*

Linear programming formulation

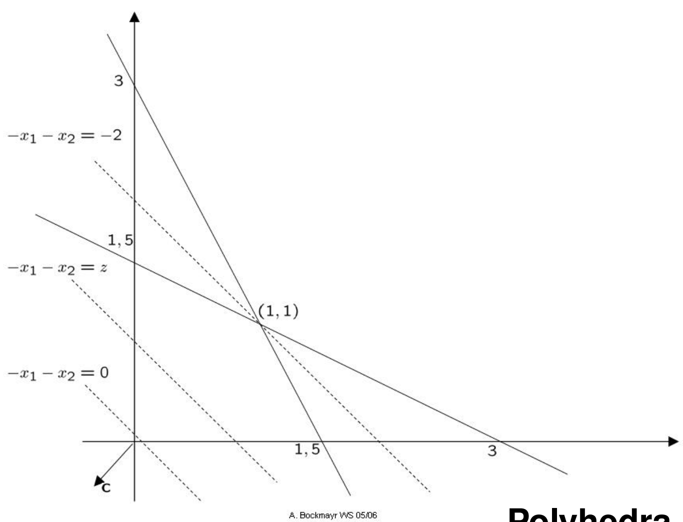
$$
\begin{array}{llcccccc}
\max & c_1x_1 & + & \cdots & + & c_nx_n & & \\
\text{w.r.t.} & a_{11}x_1 & + & \cdots & + & a_{1n}x_n & \leq & b_1, \\
 & \vdots & & & & \vdots & & \\
 & a_{m1}x_1 & + & \cdots & + & a_{mn}x_n & \leq & b_m, \\
 & x_1, & & \ldots & & ,x_n & \geq & 0.
\end{array}
$$

In matrix notation:

$$\max\{c^Tx \mid Ax \leq b, x \geq 0\},$$

where $A \in \mathbb{R}^{m\times n}, b \in \mathbb{R}^m, c \in \mathbb{R}^n, x \in \mathbb{R}^n$.

Geometric illustration



$$
\begin{array}{lccccc}
\max & x_1 & + & x_2 & & \\
\text{w.r.t.} & x_1 & + & 2x_2 & \leq & 3 \\
 & 2x_1 & + & x_2 & \leq & 3 \\
 & x_1 & , & x_2 & \geq & 0
\end{array}
$$

Polyhedra

- *Hyperplane* $H = \{x \in \mathbb{R}^n \mid a^Tx = \beta\}$, $a \in \mathbb{R}^n \setminus \{0\}, \beta \in \mathbb{R}$
- *Closed halfspace* $\overline{H} = \{x \in \mathbb{R}^n \mid a^Tx \leq \beta\}$

- *Polyhedron* $P = \{x \in \mathbb{R}^n \mid Ax \leq b\}, A \in \mathbb{R}^{m \times n}, b \in \mathbb{R}^m$
- *Polytope* $P = \{x \in \mathbb{R}^n \mid Ax \leq b,\ l \leq x \leq u\}, l, u \in \mathbb{R}^n$
- *Polyhedral cone* $P = \{x \in \mathbb{R}^n \mid Ax \leq 0\}$

The feasible set

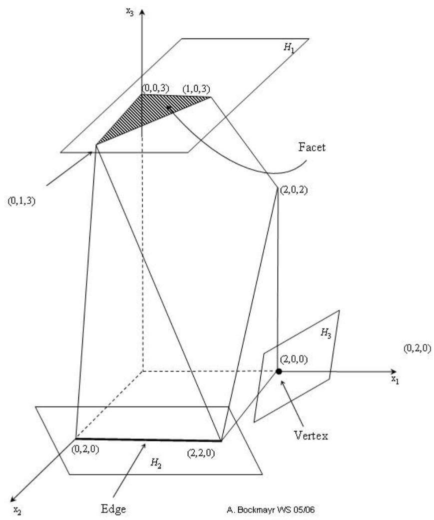
$$P = \{x \in \mathbb{R}^n \mid Ax \leq b\}$$

of a linear optimization problem is a polyhedron.

Vertices, Faces, Facets

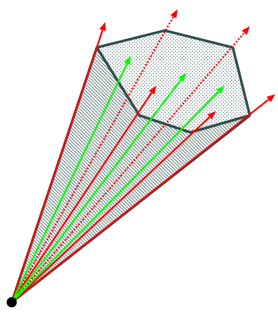
- $P \subseteq \overline{H}, H \cap P \neq \emptyset$ *(Supporting hyperplane)*
- $F = P \cap H$ *(Face)*
- $\dim(F) = 0$ *(Vertex)*
- $\dim(F) = 1$ *(Edge)*
- $\dim(F) = \dim(P) - 1$ *(Facet)*
- *P pointed:* P has at least one vertex.

Illustration



Rays and extreme rays

- $r \in \mathbb{R}^n$ is a *ray* of the polyhedron P if for each $x \in P$ the set $\{x + \lambda r \mid \lambda \geq 0\}$ is contained in P.
- A ray r of P is *extreme* if there do not exist two linearly independent rays r^1, r^2 of P such that $r = \frac{1}{2}(r^1 + r^2)$.



Hull operations

- $x \in \mathbb{R}^n$ is a *linear combination* of $x^1, \ldots, x^k \in \mathbb{R}^n$ if

$$x = \lambda_1 x^1 + \cdots + \lambda_k x^k, \text{ for some } \lambda_1, \ldots, \lambda_k \in \mathbb{R}.$$

- If, in addition

$$\left\{ \begin{array}{ll} \lambda_1, \ldots, \lambda_k \geq 0, & \\ & \lambda_1 + \cdots + \lambda_k = 1, \\ \lambda_1, \ldots, \lambda_k \geq 0, & \lambda_1 + \cdots + \lambda_k = 1, \end{array} \right\} x \text{ is a } \left\{ \begin{array}{c} \textit{conic} \\ \textit{affine} \\ \textit{convex} \end{array} \right\} \text{combination.}$$

- For $S \subseteq \mathbb{R}^n, S \neq \emptyset$, the set $\text{lin}(S)$ (resp. $\text{cone}(S), \text{aff}(S), \text{conv}(S)$) of all linear (resp. conic, affine, convex) combinations of finitely many vectors of S is called the *linear (resp. conic, affine, convex) hull of S*.

Outer and inner descriptions

- A subset $P \subseteq \mathbb{R}^n$ is a *H-polytope,* i.e., a *bounded* set of the form *Outer*

$$P = \{x \in \mathbb{R}^n \mid Ax \leq b\}, \text{ for some } A \in \mathbb{R}^{m \times n}, b \in \mathbb{R}^m.$$

  if and only if it is a *V-polytope,* i.e., *Inner*

$$P = \text{conv}(V), \text{ for some finite } V \subset \mathbb{R}^n$$

- A subset $C \subseteq \mathbb{R}^n$ is a *H-cone,* i.e., *Outer*

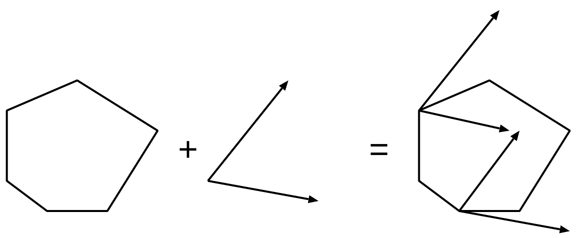
$$C = \{x \in \mathbb{R}^n \mid Ax \leq 0\}, \text{ for some } A \in \mathbb{R}^{m \times n}.$$

  if and only if it is a *V-cone,* i.e., *Inner*

$$C = \text{cone}(Y), \text{ for some finite } Y \subset \mathbb{R}^n$$

Minkowski sum

- $X, Y \subseteq \mathbb{R}^n$
- $X + Y = \{x + y \mid x \in X, y \in Y\}$ *(Minkowski sum)*



Main theorem for polyhedra

A subset $P \subseteq \mathbb{R}^n$ is a *H-polyhedron,* i.e., *Outer*

$$P = \{x \in \mathbb{R}^n \mid Ax \leq b\}, \text{ for some } A \in \mathbb{R}^{m \times n}, b \in \mathbb{R}^m.$$

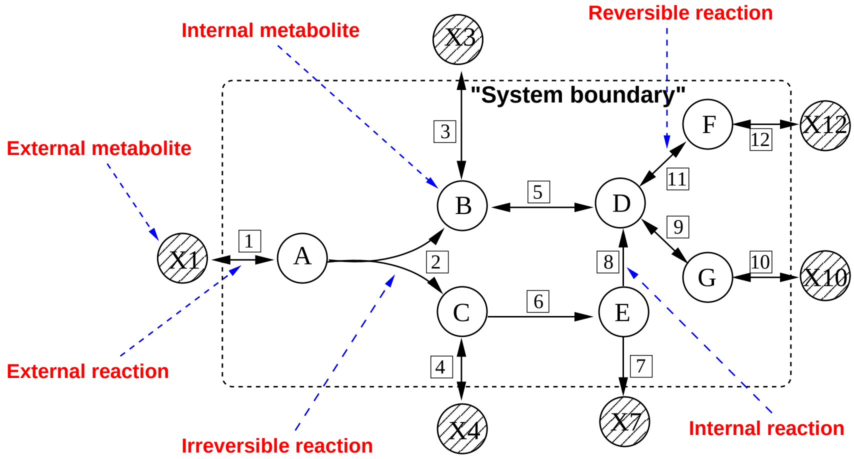
if and only if it is a *V-polyhedron,* i.e., *Inner*

$$P = \text{conv}(V) + \text{cone}(Y), \text{ for some finite } V, Y \subset \mathbb{R}^n$$

Theorem of Minkowski

- For each polyhedron $P \subseteq \mathbb{R}^n$ there exist finitely many points $p^1,\dots,p^k$ in P and finitely many rays $r^1,\dots,r^l$ of P such that
$$P = \mathrm{conv}(p^1,\dots,p^k) + \mathrm{cone}(r^1,\dots,r^l).$$
- If the polyhedron P is pointed, then $p^1,\dots,p^k$ may be chosen as the uniquely determined vertices of P, and $r^1,\dots,r^l$ as representatives of the up to scalar multiplication uniquely determined extreme rays of P.
- *Special cases*
  - A polytope is the convex hull of its vertices.
  - A pointed polyhedral cone is the conic hull of its extreme rays.

Application: Metabolic networks

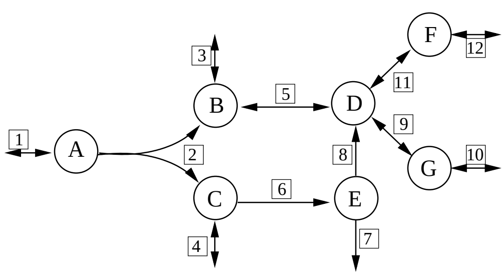


Stoichiometric matrix

- Metabolites (internal) $\leadsto$ rows
- Biochemical reactions $\leadsto$ columns

$$kA + lC \xrightarrow{j} mE + nH \qquad \begin{array}{c} A \\ B \\ C \\ D \\ E \\ F \\ G \\ H \end{array} \begin{pmatrix} \dots & -k & \dots \\ & 0 & \\ & -l & \\ & 0 & \\ & m & \\ & 0 & \\ & 0 & \\ \dots & n & \dots \end{pmatrix}$$

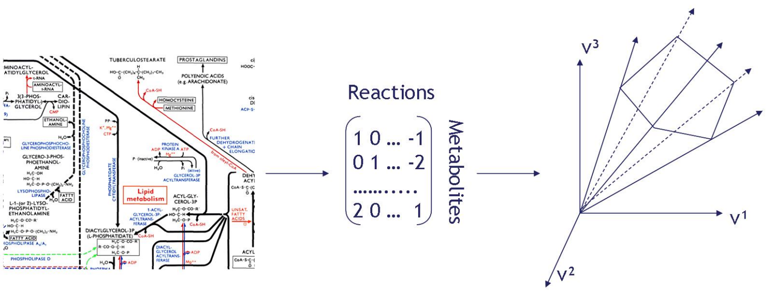
Example network



$$S = \begin{pmatrix} 1 & -1 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 \\ 0 & 1 & -1 & 0 & -1 & 0 & 0 & 0 & 0 & 0 & 0 & 0 \\ 0 & 1 & 0 & -1 & 0 & -1 & 0 & 0 & 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 & 1 & 0 & 0 & 1 & -1 & 0 & -1 & 0 \\ 0 & 0 & 0 & 0 & 0 & 1 & -1 & -1 & 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 1 & -1 \\ 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 1 & -1 & 0 & 0 \end{pmatrix}.$$

Flux cone

- Flux balance: $Sv = 0$
- Irreversibiliy of some reactions: $v_i \geq 0, i \in Irr$.
- *Steady-state flux cone*
$$C = \{v \in \mathbb{R}^n \mid Sv = 0, v_i \geq 0, \text{ for } i \in Irr\}$$
- *Metabolic network analysis* $\rightsquigarrow$ find $p^1, \ldots, p^k \in C$ with $C = \text{cone}\{p^1, \ldots, p^k\}$.



Simplex Algorithm: Geometric view

Linear optimization problem

$$\max\{c^T x \mid Ax \leq b, x \in \mathbb{R}^n\} \tag{LP}$$

Simplex-Algorithm (Dantzig 1947)

1. Find a vertex of P.
2. Proceed from vertex to vertex along edges of P such that the objective function $z = c^T x$ increases.
3. Either a vertex will be reached that is optimal, or an edge will be chosen which goes off to infinity and along which z is unbounded.

Basic solutions

- $Ax \leq b$, $A \in \mathbb{R}^{m \times n}, rank(A) = n$.
- $M = \{1, \ldots, m\}$ row indices, $N = \{1, \ldots, n\}$ column indices
- For $I \subseteq M, J \subseteq N$ let A_{IJ} denote the submatrix of A defined by the rows in I and the columns in J.
- $I \subseteq M, |I| = n$ is called a *basis of A* iff $A_{I*} = A_{IN}$ is non-singular.
- In this case, $A_{I*}^{-1} b_I$, where b_I is the subvector of b defined by the indices in I, is called a *basic solution.*
- If $x = A_{I*}^{-1} b_I$ satisfies $Ax \leq b$, then x called a *basic feasible solution* and I is called a *feasible basis.*

Algebraic characterization of vertices

Theorem

Given the non-empty polyhedron $P = \{x \in \mathbb{R}^n \mid Ax \leq b\}$, where rank($A$) = n, a vector $v \in \mathbb{R}^n$ is a vertex of P if and only if it is a basic feasible solution of $Ax \leq b$, for some basis I of A.

For any $c \in \mathbb{R}^n$, either the maximum value of $z = c^T x$ for $x \in P$ is attained at a vertex of P or z is unbounded on P.

Corollary

P has at least one and at most finitely many vertices.

Remark

In general, a vertex may be defined by several bases.

Simplex Algorithm: Algebraic version

- Suppose rank(A) = n (otherwise apply Gaussian elimination).
- Suppose I is a feasible basis with corresponding vertex $v = A_{I*}^{-1} b_I$.
- Compute $u^T \stackrel{\text{def}}{=} c^T A_{I*}^{-1}$ (vector of n components indexed by I).
- If $u \geq 0$, then v is an optimal solution, because for each feasible solution x

$$c^T x = u^T A_{I*} x \leq u^T b_I = u^T A_{I*} v = c^T v.$$

- If $u \not\geq 0$, choose $i \in I$ such that $u_i < 0$ and define the direction $d \stackrel{\text{def}}{=} -A_{I*}^{-1} e_i$, where e_i is the i-th unit basis vector in $\mathbb{R}^I$.
- Next increase the objective function value by going from v in direction d, while maintaining feasibility.

Simplex Algorithm: Algebraic version (2)

1. If $Ad \not\leq 0$, the largest $\lambda \geq 0$ for which $v + \lambda d$ is still feasible is

$$\lambda^* = \min\{\frac{b_l - A_{l*} v}{A_{l*} d} \mid l \in \{1, \dots, m\}, A_{l*} d > 0\}. \quad \text{(PIV)}$$

   Let this minimum be attained at index k. Then $k \notin I$ because $A_{I*} d = -e_i \leq 0$.

   Define $I' = (I \setminus \{i\}) \cup \{k\}$, which corresponds to the vertex $v + \lambda^* d$.

   Replace I by I' and repeat the iteration.

2. If $Ad \leq 0$, then $v + \lambda d$ is feasible, for all $\lambda \geq 0$. Moreover,

$$c^T d = -c^T A_{I*}^{-1} e_i = -u^T e_i = -u_i > 0.$$

   Thus the objective function can be increased along d to infinity and the problem is unbounded.

Termination and complexity

- The method terminates if the indices i and k are chosen in the right way (such choices are called *pivoting rules*).

- Following the rule of Bland, one can choose the smallest i such that $u_i < 0$ and the smallest k attaining the minimum in (PIV).
- For most known pivoting rules, sequences of examples have been constructed such that the number of iterations is exponential in $m+n$ (e.g. Klee-Minty cubes).
- Although no pivoting rule is known to yield a polynomial time algorithm, the Simplex method turns out to work very well in practice.

Simplex : Phase I

- In order to find an *initial feasible basis*, consider the auxiliary linear program

$$\max\{y \mid Ax - by \leq 0,\ \ -y \leq 0,\ \ y \leq 1\}, \tag{Aux}$$

  where y is a new variable.
- Given an arbitrary basis K of A, obtain a feasible basis I for (Aux) by choosing $I = K \cup \{m+1\}$. The corresponding basic feasible solution is 0.
- Apply the Simplex method to (Aux). If the optimum value is 0, then (LP) is infeasible. Otherwise, the optimum value has to be 1.
- If I' is the final feasible basis of (Aux), then $K' = I' \setminus \{m+2\}$ can be used as an initial feasible basis for (LP).

Duality

- *Primal problem:* $z_P = \max\{\mathbf{c}^\mathsf{T} x \mid Ax \leq b,\ x \in \mathbb{R}^n\}$ (P)
- *Dual problem:* $w_D = \min\{b^T u \mid A^T u = \mathbf{c},\ u \geq 0\}$ (D)

General form

(P)			(D)		
min	$c^T x$		max	$u^T b$	
w.r.t.	$A_{i*}x \geq b_i$,	$i \in M_1$	w.r.t.	$u_i \geq 0$,	$i \in M_1$
	$A_{i*}x \leq b_i$,	$i \in M_2$		$u_i \leq 0$,	$i \in M_2$
	$A_{i*}x = b_i$,	$i \in M_3$		u_i free,	$i \in M_3$
	$x_j \geq 0$,	$j \in N_1$		$(A_{*j})^T u \leq c_j$,	$j \in N_1$
	$x_j \leq 0$,	$j \in N_2$		$(A_{*j})^T u \geq c_j$,	$j \in N_2$
	x_j free,	$j \in N_3$		$(A_{*j})^T u = c_j$,	$j \in N_3$

Duality theorems

Theorem

- If x^* is primal feasible and u^* is dual feasible, then

$$c^T x^* \leq z_P \leq w_D \leq b^T u^*.$$

- Only four possibilities:
  1. z_P and w_D are both finite and equal.
  2. $z_P = +\infty$ and (D) is infeasible.

3. $w_D = -\infty$ and (P) is infeasible.
4. (P) and (D) are both infeasible.

Complexity of linear programming

Theorem (Khachyian 79)
The following problems are solvable in polynomial time:

- Given a matrix $A \in \mathbb{Q}^{m \times n}$ and a vector $b \in \mathbb{Q}^m$, decide whether $Ax \leq b$ has a solution $x \in \mathbb{Q}^n$, and if so, find one.
- (Linear programming problem) Given a matrix $A \in \mathbb{Q}^{m \times n}$ and vectors $b \in \mathbb{Q}^m, c \in \mathbb{Q}^n$, decide whether $\max\{c^T x \mid Ax \leq b, x \in \mathbb{Q}^n\}$ is infeasible, finite, or unbounded. If it is finite, find an optimal solution. If it is unbounded, find a feasible solution x_0, and find a vector $d \in \mathbb{Q}^n$ with $Ad \leq 0$ and $c^T d > 0$.

Complexity of integer linear programming

Satisfiability	over $\mathbb{Q}$	over $\mathbb{Z}$	over $\mathbb{N}$
Linear equations	polynomial	polynomial	NP-complete
Linear inequalities	polynomial	NP-complete	NP-complete